CONTENTS

Part I
Committees, Sponsors vi
Preface vii
Physical properties in chemical process design—past, present, future
H. Knapp (Berlin, F.R.G.) 1

Process Design and Simulation Needs
A review of thermophysical properties in process simulation
J.T. Adams (Houston, TX, U.S.A.) 23
Data quality for process design
A.H. Larsen (St. Louis, MO, U.S.A.) 47
Exact determination of process sensitivity to physical properties
S. Macchietto, G. Maduabeuke, R. Szczepanski (London, Gt. Britain) 59
Industrial applications of UNIFAC
C. Torres-Marchal and A.L. Cantalino (Camaçari, Brazil) 69
Process design needs in oil and gas offshore industry
T. Saeterstad (Trondheim, Norway) 77
Fluid properties in reservoir simulation
V. Dalen (Stavanger, Norway) 93
The processing of biomacromolecules: a challenge for the Eighties
R.D. Johnson (West Point, PA, U.S.A.) 109
A strategy for the design and selection of solvents for separation processes
E.A. Brignole, S. Bottini and R. Gani (Bahia Blanca, Argentina) 125
Supercritical fluid extraction
E.A. Brignole (Bahia Blanca, Argentina) 133

Experimental Methods
High pressure phase equilibria: experimental methods
U.K. Deiters and G.M. Schneider (Bochum, F.R.G.) 145
High pressure PVT measurements
J.C. Holste, K.R. Hall, P.T. Eubank, K.N. Marsh (College Station, TX, U.S.A.) 161
Recent advances in calorimetry
Wm.R. Parrish (Bartlesville, OK, U.S.A.) 177
Low-pressure phase equilibria: measurement of VLE
M.M. Abbott (Troy, NY, U.S.A.) 193
The occurrence and measurement of multiphase equilibria behavior
K.D. Luks (Tulsa, OK, U.S.A.) 209
Measurement of vapor–liquid equilibria at elevated temperatures and pressures using a flow type apparatus
H. Inomata, K. Arai and S. Saito (Sendai, Japan) 225
An experimental method for the measurement of the two-phase liquid hydrocarbon–hydrate equilibrium
E.D. Sloan, M.S. Bourrie, K.A. Sparks and J.J. Johnson (Golden, CO, U.S.A.) 233
Design of a differential pressure cell, VLE of aldehyde systems and new UNIFAC parameters
K.-D. Kassmann and H. Knapp (Berlin, F.R.G.) 241

A differential static apparatus for the investigation of the infinitely diluted region
P. Alessi, M. Fermeglia and I. Kikic (Trieste, Italy) 249
VLE and LLE in binary 2-methoxyethanol–alkane systems
E. Dolch, A. Matovu and R.N. Lichtenthaler (Heidelberg, F.R.G.) 257
Experimental solid–liquid equilibria of binary mixtures of organic compounds
P.C. Proust and J.C. Fernandez (Valparaiso, Chile) 265
The transient total pressure method: An analysis
C.S. Howat (Lawrence, KS, U.S.A.) 273

Molecular Simulation, Polymer Solutions and Surface Tension
Molecular simulation: progress and prospects
N. Quirke (Sunbury-on-Thames, Gt. Britain) 283
Computer simulation of fluid mixtures
J.M. Haile (Clemson, SC, U.S.A.) 307
Monte-Carlo simulation of continuous Lennard–Jones mixtures
D.A. Kofke and E.D. Glandt (Philadelphia, PA, U.S.A.) 327
Theory and simulation of associating liquid mixtures
W.G. Chapman and K.E. Gubbins (Ithaca, NY, U.S.A.), C.G. Joslin and C.G. Gray (Guelph, Ontario, Canada) 337
PVT relation and density-dependent local composition for supercritical and subcritical fluid mixtures of Lennard–Jones molecules
K. Nakanishi (Kyoto, Japan), Y. Adachi (Nagoya, Japan) and I. Fujihara (Osaka, Japan) 347
Phase equilibria in polymer solutions by group contribution
J. Holten-Andersen, Aa. Fredenslund, P. Rasmussen and G. Carvoli (Lyngby, Denmark) 357
Aqueous polymer two-phase systems in biotechnology
Å. Gustafsson, H. Wennerström and F. Tjerneld (Lund, Sweden) 365
Fractionation of polymers with supercritical fluids
S.K. Kumar, U.W. Suter, R.C. Reid (Cambridge, MA, U.S.A.) 373
Surface tension: a simple correlation for natural gas + condensate systems
J.A. Hugill and A.J. Van Welsenes (Amsterdam, The Netherlands) 383

High-Pressure Phase Equilibria
High-pressure vapor–liquid equilibria with cubic equations of state
C. Tsonopoulos and J.L. Heidman (Florham Park, NJ, U.S.A.) 391
Density dependent local composition models: an interpretive review
R.P. Danner and P.A. Gupte (University Park, PA, U.S.A.) 415
A cubic equation of state for polar and other complex mixtures
J.O. Valderrama (Dhahran, Saudi Arabia) and L.A. Cisternas (Antofagasta, Chile) 431
Correlation of ammonia–water equilibrium data with various modified Peng–Robinson equations of state
R.A. Heidemann and S.S.H. Rizvi (Calgary, Alberta, Canada) 439
Phase behavior in fluid–solid systems
G.D. Holder (Pittsburgh, PA, U.S.A.) 447
A practical extension of equations of state to polar systems
H. Ozkardesh (Houston, TX, U.S.A.) 457
Accuracy and consistency comparisons of ten cubic equations of state for polar and non-polar compounds
M.A. Trebble and P.R. Bishnoi (Calgary, Alberta, Canada) 465
Cubic chain-of-rotators equation of state with density-dependent local composition mixing rules
R.J. Lee and K.C. Chao (West Lafayette, IN, U.S.A.) 475
Equation of state mixing rules from G^E models
P.A. Gupte, P. Rasmussen and Aa. Fredenslund (Lyngby, Denmark) 485

Three phase equilibria in binary mixtures of ethane and higher n-alkanes
C.J. Peters, R.N. Lichtenthaler and J. de Swaan Arons (Delft, The Netherlands) 495
Fluid phase equilibria in the binary systems ethylene + n-triacontane and ethylene + squalane
Th.W. de Loos, W. Poot and J. de Swaan Arons (Delft, The Netherlands) 505
Multiphase equilibria in high-pressure ternary systems containing secondary alcohols and water
M. Radosz (Annandale, NJ, U.S.A.) 515
Multiphase high pressure equilibria in ternary aqueous systems
A.Z. Panagiotopoulos and R.C. Reid (Cambridge, MA, U.S.A.) 525
Phase equilibria in ternary and quaternary systems of hydrogen, water and hydrocarbons at elevated temperatures and pressures
R. Dohrn and G. Brunner (Hamburg, F.R.G.) 535
Phase equilibria for supercritical extraction of lemon flavours and palm oils with carbon dioxide
P.M. Mathias, T.W. Copeman and J.M. Prausnitz (Allentown, PA, U.S.A.) 545
High pressure phase equilibria for binary systems involving a solid phase
P.L. Cheong, Dingan Zhang, K. Ohgaki and B.C.-Y. Lu (Ottawa, Ontario, Canada) 555
Phase equilibria for a rich gas condensate–nitrogen system
R.S. Metcalfe and W.J. Raby (Tulsa, OK, U.S.A.) 563
Prediction of properties of petroleum mixtures: improvement in reliability and validity of tuned parameters
R. Gani and Aa. Fredenslund (Lyngby, Denmark) 575
Vapor–liquid equilibrium calculations with the BACK equation of state
K. Aim and T. Boublik 583
Author Index 593

Part II
Critical phenomena and computation methods
Some theoretical aspects of critical phenomena in fluids
B. Widom and G. Sundar (Ithaca, NY, U.S.A.) 1
Some aspects of multiphase calculations
M.L. Michelsen (Lyngby, Denmark) 15
Dilute mixtures and solutions near critical points
J.M.H. Levelt Sengers (Gaithersburg, MD, U.S.A.) 31
A decorated lattice-gas model of supercritical fluid solubilities and partial molar volumes
S.W. Gilbert and C.A. Eckert (Urbana, IL, U.S.A.) 41
Saturated phase equilibria and parameter estimation of pure fluids with two lattice-gas model
P.K. Kilpatrick and Shu-Hua Chang (Raleigh, NC, U.S.A.) 49
Phase equilibrium computational algorithms of continuous mixtures
P.C. Du and G. Ali Mansoori (Chicago, IL, U.S.A.) 57
Phase equilibria in oleochemical industry—application of continuous thermodynnamics
B. Gutsche (Düsseldorf, F.R.G.) 65
Adiabatic flash calculations for continuous or semicontinuous mixtures using an equation of state
G.F. Chou and J.M. Prausnitz (Berkeley, CA, U.S.A.) 75
Phase equilibria and chemical reaction
A.E. Mather (Edmonton, Alberta, Canada) 83

Evaluation of methods for calculating liquid–liquid phase-splitting
D.J. Swank and J.C. Mullins (Clemson, SC, U.S.A.) 101
The application of fuzzy set theory to uncertainty in physical property models
W.L. Kubic, Jr. and F.P. Stein (Bethlehem, PA, U.S.A.) 111

Phase Equilibria in Complex Mixtures
Group contribution methods for the estimation of activity coefficients
J. Gmehling (Dortmund, F.R.G.) 119
A proper theoretical basis for local composition mixing rules and a new class of activity coefficients models
S.I. Sandler and Kun-Hong Lee (Newark, DL, U.S.A.) 135
Integral equation group contribution methods
P.D. McMahon (Madison, WI, U.S.A.) 143
Prediction of viscosities of liquid mixtures by a group contribution method
D.T. Wu (Philadelphia, PA, U.S.A.) 149
Thermodynamics of complex aqueous systems
J.P.E. Grolier, G. Roux-Desgranges and A.H. Roux (Aubière, France) 157
The pseudo-phase analogy: application of vapor–liquid equilibria techniques to micellar solutions
K.R. Cox and H.L. Benson (Houston, TX, U.S.A.) 173
Electrolyte solutions
H. Renon (Paris, France) 181
An equation of state description of weak electrolyte VLE behavior
K.J. Daumn, B.K. Harrison, D.B. Manley, B.E. Poling (Rolla, MO, U.S.A.) 197
A fluctuation theory model of strong electrolytes
H. Cabezas, Jr. and J.P. O'Connell (Gainesville, FL, U.S.A.) 213
Prediction of Henry's constants of gases in electrolyte solutions
Y.N. Xu and Y. Hu (Shanghai, People's Republic of China) 221
Prediction of brine process chemistry from theoretical models
N. Møller and J.H. Weare (La Jolla, CA, U.S.A.) 229
An explicit non-equal diameter MSA model for electrolytes
T.W. Copeman (Allentown, PA, U.S.A.) and F.P. Stein (Bethlehem, PA, U.S.A.) 237
Phase equilibria in natural gas, crude oil and coal liquid mixtures
A.S. Teja and B.T. Willman (Atlanta, GE, U.S.A.) 247
Dew points of wet gas mixtures: new data and a new correlation using interaction third virial coefficients
P.T. Eubank, J.J. Scheloske, L.L. Joffrion (College Station, TX, USA) 255
Thermodynamics for solid solution–liquid–vapor equilibria: wax phase formation from heavy hydrocarbon mixtures
K.W. Won (Irvine, CA, U.S.A.) 265
Pseudo-critical properties of heavy oils and bitumens
Cheng-Tze Fu, R. Puttagunta, L. Baumber and Chu Hsi (Edmonton, Alberta, Canada) . 281
A study on scatchard–Hildebrand solution theory for metal solvent extraction systems
Yi-Gui Li, Teng Teng, Jiu-Fang Lu, Gang Chen and Ji-Ding Li (Beijing, People's Republic of China) 297
Phase equilibrium predictions for polar and hydrogen bonding mixtures
M.D. Donohue, P. Vilmalchand and G.D. Ikonomou (Baltimore, MD, U.S.A.) 307
Unified model of associated solutions (UMAS)
F. Aguirre-Ode (Valparaiso, Chile) 315
A generalized description of multiple phase behavior in isothermal, isobaric systems
D.J. Mangone, R.M. Enick and G.D. Holder (Pittsburgh, PA, U.S.A.) 327

Future Problems
Phase equilibria in chemically reactive systems
G. Maurer (Kaiserlautern, F.R.G.) 337
Structural characterization and property estimation for complex mixtures
D.T. Allen (Los Angeles, CA, U.S.A.) 353
Phase behavior of flowing polymer mixtures
M. Tirrell (Minneapolis, MN, U.S.A.) 367
Author Index 381